EFFECTIVE FIELD THEORY FOR PHASE TRANSITION OF PROTEIN MACRO-MOLECULE INDUCED BY FORCE

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In the framework of the effective field theory for the order parameter, which characterizes the degree of deviating the protein globule structure from its native state, the phase transition of the protein macromolecule from the elastic state into the plastic one under its mechanical stretching is considered. Elastic properties of a protein are studied as a function of the applied force, temperature and the mean coordination number of the protein "network".

Recently the methods to investigate protein unfolding at the single-molecule level have been developed. In particular, in experiments on the mechanical unfolding of proteins the external force F is applied between a pair of amino-acid residues and the dependence of the distance x between them is measured as a function of the force.

Dependencies $x(F)$ of the single protein molecule extension on the applied force demonstrate some "fine structure", associated with successive ruptures of individual bonds between residues. However, broadly speaking, one could reveal that all those dependencies have some general feature − each of them demonstrates the saturation: when the force becomes strong enough the protein begins to "flow", that is to lengthen rapidly without further growth of the applied force. It seems as though the sharp (phase?) transition occurs under which the protein "skeleton" loses the stability and transits from the elastic state into the plastic one.

Our aim is to describe analytically the process of protein mechanical unfolding. To this end, we investigate the hypothetic protein phase transition in terms of graph (network) theory which, putting aside the nature of interacting elements composing the network, describes general features of such systems, allows to classify them by certain characteristics, to estimate qualitatively their stability, etc. We have studied (in the framework of the effective field theory) the phase transition of a protein macromolecule from the elastic state to the plastic one, which arises from mechanical stretching.

With increasing the stretching force the sharp drop of the protein elasticity occurs, it losses the rigidity, and the protein begins to "flow" freely. Near that threshold, the rigidity falls according to the percolation theory. The critical force depends significantly on the average number of bonds for amino-acid residues in a protein. Protein networks with average coordination number smaller than some critical value could not exist in the globular state − arbitrarily small force destroys that state. In a whole, results agree with experiments that gives promise that the effective field theory describes integral mechanical properties of protein macromolecules quite adequately.